

# Theory of the helium isotope shift

Krzysztof Pachucki

*Institute of Theoretical Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland*

V. A. Yerokhin

*Center for Advanced Studies, St. Petersburg State Polytechnical University,  
Polytekhnicheskaya 29, St. Petersburg 195251, Russia*

Theory of the isotope shift of the centroid energies of light few-electron atoms is reviewed. Numerical results are presented for the isotope shift of the  $2^3P-2^3S$  and  $2^1S-2^3S$  transition energies of  $^3\text{He}$  and  $^4\text{He}$ . By comparing theoretical predictions for the isotope shift with the experimental results, the difference of the squares of the nuclear charge radii of  $^3\text{He}$  and  $^4\text{He}$ ,  $\delta R^2$ , is determined with high accuracy.

## I. INTRODUCTION

Helium is the simplest few-electron atom that can be calculated *ab initio* [1] and measured with a very high accuracy. Optical measurements in  $^3\text{He}$  [2, 3] and  $^4\text{He}$  [4] has recently reached the relative precision of few parts in  $10^{-12}$ . Such measurements are sensitive to the nuclear size effect on the level of  $10^{-4}$ . They are approaching the level that might allow an improved determination of the Rydberg constant, which is currently considered as the one of the best known fundamental constants [5]. The accuracy of the present-day experiments is high enough for an accurate spectroscopic determination of the nuclear charge radii of  $^3\text{He}$  and  $^4\text{He}$ . Such determination would be of particular interest in view of the discrepancy for the proton charge radius observed in the muonic hydrogen experiment [6, 7]. The follow-up experiment on the muonic helium [8] might soon bring the charge radius of helium into focus.

Unfortunately, the present-day theory of the energy levels in helium [9, 10] is not good enough to provide the nuclear charge radii of  $^3\text{He}$  and  $^4\text{He}$  with the required precision. A more feasible task at present is the high-precision determination of the nuclear charge radii difference of these isotopes, which is extracted from the isotope shift of the transition energies. In the current paper we make a review of the theory of the isotope shift in light few-electron atoms, describe our calculation of the isotope shift for helium, and determine the difference of the squares of the nuclear charge radii of  $^3\text{He}$  and  $^4\text{He}$ ,  $\delta R^2$ . The results of the  $\delta R^2$  determination have already been published in Ref. [3]. In this work we present details of the calculation and the underlying theory.

We define the *isotope shift* of two isotopes as the difference of the centroid energies. More specifically, we are presently interested in the centroid energies of the  $2P$  and  $2S$  states, which are defined as an average over all fine and hyperfine energy sublevels,

$$E(2^{2S+1}L) = \frac{\sum_{J,F} (2F+1) E(2^{2S+1}L_{J,F})}{(2I+1)(2S+1)(2L+1)}, \quad (1)$$

where  $2^{2S+1}L$  denotes the state with the angular momentum  $L$  and the spin  $S$ . This definition of the isotope

shift differs from the definition sometimes used previously (e.g., in Refs. [1, 2, 11]) by the fact that we average out not only the hyperfine but also the fine-structure splitting. The advantage of using the centroid energy is that its theory is much more transparent than that of the individual sublevels  $2^{2S+1}L_{J,F}$ . Moreover, the centroid transition energy can be directly accessed in an experiment, by measuring all independent fine and hyperfine transitions and averaging them out.

Theory of the isotope shift is much simpler than theory of the energy levels because only very restricted set of operators contribute to it. Specifically, only the operators that depend on the nuclear mass or the nuclear size contribute to the isotope shift. In addition, due to the averaging over the fine and hyperfine energy sublevels in (1), all operators that depend the nuclear or the electron spin do not (almost) contribute to the isotope shift. More exactly, such operators contribute only through the second-order perturbations, most of which are negligible at the level of the present interest.

## II. THEORY

Within the nonrelativistic QED approach, energy levels of atoms are represented by an expansion in powers of the fine-structure constant  $\alpha$ ,

$$E(\alpha) = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + \dots, \quad (2)$$

where  $E^{(n)} \equiv m\alpha^n \mathcal{E}^{(n)}$  is a contribution of order  $\alpha^n$  and may include powers of  $\ln \alpha$ . Each of  $\mathcal{E}^{(n)}$  is in turn expanded in powers of the electron-to-nucleus mass ratio  $m/M$

$$\mathcal{E}^{(n)} = \mathcal{E}_{\infty}^{(n)} + \mathcal{E}_M^{(n)} + \mathcal{E}_{M^2}^{(n)} + \dots, \quad (3)$$

where  $\mathcal{E}_M^{(n)}$  denotes the correction of first order in  $m/M$  and  $\mathcal{E}_{M^2}^{(n)}$  is the second-order correction. For the description of the isotope shift, we need only the part that depends on the nuclear mass  $M$ , i.e., corrections  $\mathcal{E}_M^{(n)}$ ,  $\mathcal{E}_{M^2}^{(n)}$ , etc.

### A. Nonrelativistic recoil

The leading term in the expansion (2) is the nonrelativistic energy  $E^{(2)}$ , which is the eigenvalue of the nonrelativistic Hamiltonian,

$$H_M^{(2)} = \frac{\vec{P}^2}{2M} + \sum_a \frac{\vec{p}_a^2}{2m} - \sum_a \frac{Z}{r_a} + \sum_{a<b} \frac{1}{r_{ab}} \quad (4)$$

where  $Z$  and  $\vec{P}$  are the nuclear charge and momentum, respectively; the indexes  $a$  and  $b$  numerate the electrons,  $\vec{p}_a$  is the momentum of the electron  $a$ ,  $r_a$  is the distance between the electron  $a$  and the nucleus and  $r_{ab}$  is the radial distance between the electrons  $a$  and  $b$ .

Assuming that the total momentum is zero,

$$\vec{P}^2 = \left( -\sum_a \vec{p}_a \right)^2 = \sum_a \vec{p}_a^2 + 2 \sum_{a<b} \vec{p}_a \cdot \vec{p}_b, \quad (5)$$

and rescaling momenta and position operators in units of the reduced mass  $\mu = mM/(m+M)$ ,  $\vec{p}_a \rightarrow \mu \vec{p}_a$  and  $\vec{r}_a \rightarrow \vec{r}_a/\mu$ , the Hamiltonian  $H_M^{(2)}$  is represented as a sum of two terms,

$$H_M^{(2)} = \mu H_\infty^{(2)} + \frac{\mu^2}{m} H_{\text{rec}}^{(2)}, \quad (6)$$

with

$$H_\infty^{(2)} = \sum_a \left( \frac{\vec{p}_a^2}{2} - \frac{Z}{r_a} \right) + \sum_{a<b} \frac{1}{r_{ab}} \quad (7)$$

and

$$H_{\text{rec}}^{(2)} = \frac{m}{M} \sum_{a<b} \vec{p}_a \cdot \vec{p}_b. \quad (8)$$

The eigenvalue of  $H_\infty^{(2)}$  is  $\mathcal{E}_\infty^{(2)}$ , the nonrelativistic energy in the nonrecoil limit. In the present work we are interested in the recoil (i.e.,  $M$ -dependent) corrections to  $\mathcal{E}_\infty^{(2)}$ . The correction coming from  $\mu H_\infty^{(2)}$  is often termed as the normal mass shift. It is given by

$$\mathcal{E}_{M,0}^{(2)} = \left( \frac{\mu}{m} - 1 \right) \mathcal{E}_\infty^{(2)}. \quad (9)$$

The second recoil correction is induced by  $H_{\text{rec}}^{(2)}$ ; it is known as the specific mass shift or the mass polarization. This correction can, in principle, be calculated numerically to all orders in  $m/M$  by including  $H_{\text{rec}}^{(2)}$  into the nonrelativistic Hamiltonian, determining the corresponding eigenvalue and subtracting the nonrecoil limit  $M \rightarrow \infty$ . This approach works very well for  $P$  states but becomes numerically unstable for  $S$  states (with the basis of the fully correlated exponential functions used in the present work). Because of this, we obtain the specific mass shift corrections by perturbation theory, extending

it up to the third order. The perturbation corrections are

$$\mathcal{E}_{M,1}^{(2)} = \left( \frac{\mu}{m} \right)^2 \left\langle H_{\text{rec}}^{(2)} \right\rangle, \quad (10)$$

$$\mathcal{E}_{M,2}^{(2)} = \left( \frac{\mu}{m} \right)^3 \left\langle H_{\text{rec}}^{(2)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \right\rangle, \quad (11)$$

$$\begin{aligned} \mathcal{E}_{M,3}^{(2)} = \left( \frac{\mu}{m} \right)^4 & \left[ \left\langle H_{\text{rec}}^{(2)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \right\rangle \right. \\ & \left. - \left\langle H_{\text{rec}}^{(2)} \right\rangle \left\langle H_{\text{rec}}^{(2)} \frac{1}{(\mathcal{E}_0 - H_0)'^2} H_{\text{rec}}^{(2)} \right\rangle \right], \end{aligned} \quad (12)$$

where  $H_0 \equiv H_\infty^{(2)}$  is the nonrelativistic Hamiltonian in the nonrecoil limit and  $\mathcal{E}_0 \equiv \mathcal{E}_\infty^{(2)}$  is its eigenvalue. We checked that, for  $P$  states, the perturbation expansion results are in a very good agreement with the nonperturbative treatment.

### B. Relativistic recoil

The leading relativistic correction to the energy is given by the expectation value of the Breit-Pauli Hamiltonian  $H^{(4)}$  [12]. The Breit-Pauli Hamiltonian with the full reduced-mass dependence is given by:

$$\begin{aligned} H^{(4)} = \left( \frac{\mu}{m} \right)^3 & \sum_a \left[ -\frac{\mu}{m} \frac{\vec{p}_a^4}{8} + \frac{\pi Z}{2} \delta^3(r_a) + \frac{Z}{4} \vec{\sigma}_a \cdot \frac{\vec{r}_a}{r_a^3} \times \vec{p}_a \right] \\ & + \left( \frac{\mu}{m} \right)^3 \sum_{a<b} \left\{ -\pi \delta^3(r_{ab}) - \frac{1}{2} \vec{p}_a^i \left( \frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i r_{ab}^j}{r_{ab}^3} \right) \vec{p}_b^j \right. \\ & - \frac{2\pi}{3} \vec{\sigma}_a \cdot \vec{\sigma}_b \delta^3(r_{ab}) + \frac{\sigma_a^i \sigma_b^j}{4r_{ab}^3} \left( \delta^{ij} - 3 \frac{r_{ab}^i r_{ab}^j}{r_{ab}^2} \right) \\ & + \frac{1}{4r_{ab}^3} [2 (\vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_a) \\ & \left. + (\vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_a)] \right\}, \end{aligned} \quad (13)$$

where  $\vec{\sigma}_a$  is the vector of Pauli  $\sigma$  matrices acting on the  $a$  electron. The Breit Hamiltonian without the reduced mass dependence (i.e., with  $\mu \rightarrow m$ ) will be denoted by  $H_\infty^{(4)}$ .

We are presently interested in the recoil corrections to the Breit contribution. First of all, there is a recoil correction induced by the reduced mass in Eq. (13),

$$\mathcal{E}_{M,0}^{(4)} = \left\langle H^{(4)} - H_\infty^{(4)} \right\rangle. \quad (14)$$

The first-order recoil correction  $\mathcal{E}_{M,1}^{(4)}$  is induced by the recoil addition to the Breit Hamiltonian and the second-order perturbation correction of the non-recoil

Breit Hamiltonian  $H_\infty^{(4)}$  and the mass-polarization operator  $H_{\text{rec}}^{(2)}$ ,

$$\mathcal{E}_{M,1}^{(4)} = \left(\frac{\mu}{m}\right)^3 \left\langle H_{\text{rec}}^{(4)} \right\rangle + 2 \left(\frac{\mu}{m}\right) \left\langle H_\infty^{(4)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \right\rangle, \quad (15)$$

where the recoil addition to the Breit Hamiltonian is

$$H_{\text{rec}}^{(4)} = \frac{Zm}{2M} \sum_{ab} \left[ \frac{\vec{r}_a}{r_a^3} \times \vec{p}_b \cdot \vec{\sigma}_a - p_a^i \left( \frac{\delta^{ij}}{r_a} + \frac{r_a^i r_a^j}{r_a^3} \right) p_b^j \right]. \quad (16)$$

The first term in the above formula represents the electron-nucleus spin-orbit interaction, whereas the second term is induced by the electron-nucleus orbit-orbit interaction.

The second-order recoil correction  $\mathcal{E}_{M,2}^{(4)}$  consists of several parts,

$$\mathcal{E}_{M,2}^{(4)} = \mathcal{E}_{M,2a}^{(4)} + \mathcal{E}_{M,2b}^{(4)} + \mathcal{E}_{M,2c}^{(4)}. \quad (17)$$

The first one is the third-order perturbation correction of the non-recoil Breit Hamiltonian  $H_\infty^{(4)}$  and two mass-polarization operators  $H_{\text{rec}}^{(2)}$ ,

$$\begin{aligned} \mathcal{E}_{M,2a}^{(4)} &= 2 \left\langle H_\infty^{(4)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \right\rangle \\ &+ \left\langle H_{\text{rec}}^{(2)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_\infty^{(4)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \right\rangle \\ &- \left\langle H_\infty^{(4)} \right\rangle \left\langle H_{\text{rec}}^{(2)} \frac{1}{(\mathcal{E}_0 - H_0)'^2} H_{\text{rec}}^{(2)} \right\rangle \\ &- 2 \left\langle H_{\text{rec}}^{(2)} \right\rangle \left\langle H_\infty^{(4)} \frac{1}{(\mathcal{E}_0 - H_0)'^2} H_{\text{rec}}^{(2)} \right\rangle. \end{aligned} \quad (18)$$

The second part is the second-order perturbation correction of the recoil Breit Hamiltonian  $H_{\text{rec}}^{(4)}$  and the mass-polarization operators  $H_{\text{rec}}^{(2)}$ ,

$$\mathcal{E}_{M,2b}^{(4)} = 2 \left\langle H_{\text{rec}}^{(4)} \frac{1}{(\mathcal{E}_0 - H_0)'} H_{\text{rec}}^{(2)} \right\rangle. \quad (19)$$

The third part is the Darwin term, which reads for the  $I = 1/2$  nuclei,

$$\mathcal{E}_{M,2c}^{(4)} = \left(\frac{m}{M}\right)^2 \left\langle \frac{Z\pi}{2} \sum_a \delta(\vec{r}_a) \right\rangle. \quad (20)$$

The Darwin term is zero for spinless nuclei.

### C. QED recoil

The leading QED correction  $\mathcal{E}_\infty^{(5)}$  in the nonrecoil limit is given by [13, 14]

$$\begin{aligned} \mathcal{E}_\infty^{(5)} &= \frac{4Z}{3} \left[ \ln(Z\alpha)^{-2} + \frac{19}{30} - \ln\left(\frac{k_0}{Z^2}\right) \right] \sum_a \langle \delta^3(r_a) \rangle \\ &+ \left[ \frac{14}{3} \ln(Z\alpha) + \frac{164}{15} \right] \sum_{a < b} \langle \delta^3(r_{ab}) \rangle \\ &- \frac{14}{3} \sum_{a < b} \left\langle \frac{1}{4\pi r_{ab}^3} + \delta^3(r_{ab}) \ln Z \right\rangle, \end{aligned} \quad (21)$$

where the singular operator  $r^{-3}$  is defined by

$$\begin{aligned} \left\langle \frac{1}{r^3} \right\rangle &\equiv \lim_{a \rightarrow 0} \int d^3r \phi^*(\vec{r}) \phi(\vec{r}) \\ &\times \left[ \frac{1}{r^3} \Theta(r - a) + 4\pi \delta^3(r) (\gamma + \ln a) \right], \end{aligned} \quad (22)$$

where  $\gamma$  is the Euler constant. The Bethe logarithm is defined as

$$\ln(k_0) = \frac{\left\langle \sum_a \vec{p}_a (H_0 - \mathcal{E}_0) \ln[2(H_0 - \mathcal{E}_0)] \sum_b \vec{p}_b \right\rangle}{2\pi Z \left\langle \sum_c \delta^3(r_c) \right\rangle}. \quad (23)$$

The recoil correction  $\mathcal{E}_M^{(5)}$  consists of three parts [15],

$$\mathcal{E}_M^{(5)} = \frac{m}{M} (\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3), \quad (24)$$

where

$$\mathcal{E}_1 = -3 E_\infty^{(5)} + \frac{4Z}{3} \sum_a \langle \delta^3(r_a) \rangle - \frac{14}{3} \sum_{a < b} \langle \delta^3(r_{ab}) \rangle, \quad (25)$$

$$\begin{aligned} \mathcal{E}_2 &= Z^2 \left[ -\frac{2}{3} \ln(Z\alpha) + \frac{62}{9} - \frac{8}{3} \ln\left(\frac{k_0}{Z^2}\right) \right] \sum_a \langle \delta^3(r_a) \rangle \\ &- \frac{14 Z^2}{3} \sum_a \left\langle \frac{1}{4\pi r_a^3} + \delta^3(r_a) \ln Z \right\rangle, \end{aligned} \quad (26)$$

and  $(m/M) \mathcal{E}_3$  is the first-order perturbation of  $E_\infty^{(5)}$  due to the mass-polarization operator  $H_{\text{rec}}^{(2)}$ .

### D. Higher-order recoil corrections

The QED correction of order  $m^2 \alpha^6 / M$  was estimated by using the hydrogen results [5],

$$\begin{aligned} \mathcal{E}_{M,\text{QED}}^{(6)} &= Z^2 \pi \sum_a \langle \delta^3(r_a) \rangle \left[ \left( \frac{\mu^3}{m^3} - 1 \right) \left( \frac{427}{96} - 2 \ln 2 \right) \right. \\ &+ \frac{m}{M} \left( \frac{35}{36} - \frac{448}{27\pi^2} - 2 \ln 2 + \frac{6}{\pi^2} \zeta(3) \right) \\ &\left. + Z \frac{m}{M} \left( 4 \ln 2 - \frac{7}{2} \right) \right]. \end{aligned} \quad (27)$$

The first term in the brackets in the above equation is due to the reduced mass scaling of the  $A_{50}$  one-loop QED contribution, the second term is the radiative recoil correction, and the third term is the pure recoil contribution.

Another important correction of order  $m^2\alpha^6/M$  comes from the second-order hyperfine correction. We keep only the important part of this correction for the  $2P$  states, which is enhanced by the small  $2^3P - 2^1P$  energy difference in the denominator. This correction is referred to as the hyperfine mixing contribution and is given by, for the  $2^3P$  state,

$$E_{M,\text{hfsmix}}^{(6)} = \frac{\left| \langle 2^3P | H_{\text{hfs}}^{(4)} | 2^1P \rangle \right|^2}{E_0(2^3P) - E_0(2^1P)}, \quad (28)$$

where  $H_{\text{hfs}}^{(4)}$  is the operator responsible for the leading-order hyperfine structure splitting. In relativistic units,

$$H_{\text{hfs}}^{(4)} = \mu_B g \mu_N \vec{I} \cdot \sum_a \left[ \frac{8\pi}{3} \delta(\vec{r}_a) \vec{\sigma}_a + \frac{3\vec{r}_a (\vec{\sigma}_a \cdot \vec{r}_a) - \vec{\sigma}_a r_a^2}{r_a^5} + 2 \frac{\vec{r}_a \times \vec{p}_a}{r_a^3} \right], \quad (29)$$

where  $\mu_B = e/(2m)$  is the Bohr magneton,  $\mu_N = e/(2m_p)$  is the nuclear magneton (with  $m_p$  being the proton mass),  $g$  is the nuclear  $g$  factor, and  $\vec{I}$  is the nuclear spin. We note that the last term in Eq. (29) does not contribute to the hyperfine mixing. For the  $2^1P$  state, the hyperfine mixing contribution is given by the same expression (28) with the opposite overall sign.

### E. Nuclear polarizability

The nuclear polarizability correction to the energy levels can be represented as

$$\mathcal{E}_{\text{pol}}^{(4)} = - \sum_a \langle \delta^3(r_a) \rangle \tilde{\alpha}_{\text{pol}}. \quad (30)$$

The coefficient  $\tilde{\alpha}_{\text{pol}}$  in the above formula was evaluated [16] as  $\tilde{\alpha}_{\text{pol}}(^4\text{He}) = 2.07(20) \text{ fm}^3$  and  $\tilde{\alpha}_{\text{pol}}(^3\text{He}) = 3.56(36) \text{ fm}^3$ . Somewhat smaller values were later obtained in Ref. [17], the difference being not important at the level of interest of the present investigation.

### F. Finite nuclear size

The leading finite nuclear size (fs) correction to the centroid energy is, in relativistic units,

$$E_{\text{fs}} = \frac{2\pi}{3} m Z \alpha \left( \frac{\mu}{m} \right)^3 \frac{R^2}{\lambda_C^2} \left\langle \sum_a \delta^3(r_a) \right\rangle \times \left[ 1 - (Z\alpha)^2 \ln(Z\alpha R/\lambda_C) + (Z\alpha)^2 f_{\text{fs}} \right], \quad (31)$$

where  $R$  is the root-mean-square (rms) nuclear charge radius  $R = \sqrt{\langle R^2 \rangle}$ ,  $\lambda_C$  is the Compton wavelength divided by  $2\pi$  and  $f_{\text{fs}}$  is the nonlogarithmic relativistic and higher-order correction. The second term in the brackets in Eq. (31) is the leading logarithmic relativistic correction, known from the hydrogen theory [5]. It is state-independent and can be directly generalized to the helium case.

The nonlogarithmic relativistic correction  $f_{\text{fs}}$  is state dependent and, moreover, dependent on the nuclear model. In the present work, we estimate  $f_{\text{fs}}$  basing on the theory of  $\text{He}^+$ , where it can be obtained by a direct numerical evaluation [18]. Our calculations, performed with quadruple-precision arithmetics for the  $1s$  state of  $\text{He}^+$ , yield  $f_{\text{fs}} = -0.04$  for the Gauss nuclear model,  $f_{\text{fs}} = 0.02$  for the sphere nuclear model, and  $f_{\text{fs}} = -0.14$  for the exponential-distribution nuclear model. Basing on these results, we estimate the corresponding correction for helium as  $f_{\text{fs}} = 0.0(2)$ . The error ascribed to  $f_{\text{fs}}$  corresponds to the fractional error of  $4 \times 10^{-5}$  in  $E_{\text{fs}}$ , which is negligible at the level of the present experimental interest.

The correction beyond the mean-square charge radius  $E_Z$  comes from the two-photon exchange [19], which is, in relativistic units,

$$E_Z = -\frac{\pi}{3} m (Z\alpha)^2 \left( \frac{\mu}{m} \right)^3 \frac{\langle R^3 \rangle}{\lambda_C^3} \left\langle \sum_a \delta^3(r_a) \right\rangle. \quad (32)$$

Since it is proportional to  $\langle R^3 \rangle$  it depends on the charge distribution. However, this effect is almost negligible for light atoms, namely the ratio

$$\frac{E_Z}{E_{\text{fs}}} = -\frac{Z\alpha}{2} \frac{\langle R^3 \rangle}{\lambda_C \langle R^2 \rangle} \quad (33)$$

for He amounts to about  $4 \times 10^{-5}$ .

## III. THEORETICAL RESULTS

Our main goal in the present investigation is the determination of the difference of the nuclear charge radii from the isotope shift. To this end, we separate our theory of the isotope shift into two parts. The first part is the theory the isotope shift for the point-like nucleus. The second part is the finite nuclear size effect, which is parameterized as  $\delta E_{\text{fs}} = C R^2$ , where  $R$  is the rms nuclear charge radius and the coefficient  $C$  is calculated numerically. Now, a comparison of the experimental value with the theoretical results for the isotope shift allows us to extract the difference of the squared rms nuclear charge radii of the two isotopes.

Numerical results of our calculation of the isotope shift of the  $2^3P-2^3S$  and  $2^1S-2^3S$  transitions for the point nucleus are presented in Tables I and II, respectively. The following masses of the helion  $m_h$  and the alpha particle  $m_\alpha$  were used in the calculations

TABLE I:  ${}^3\text{He}$ – ${}^4\text{He}$  isotope shift of the  $2^1S - 2^3S$  transition, for the point-like nucleus, in kHz.

$\mu\alpha^2$	−8 632 567.86
$\mu\alpha^2 (\mu/M)$	608 175.58
$\mu\alpha^2 (\mu/M)^2$	−7 319.80
$\mu\alpha^2 (\mu/M)^3$	0.30
$\mu\alpha^4$	−8 954.22
$\mu\alpha^4 (\mu/M)$	6 458.23
$\mu\alpha^4 (\mu/M)^2$	1.84
$m\alpha^5 (m/M)$	56.61
$m\alpha^6 (m/M)$	2.75 (69)
Hfsmix	80.72
NPol	0.20 (2)
Sum	−8 034 065.66 (69)
Ref. [20] <sup>a</sup>	−8 034 067.8 (1.1)

<sup>a</sup> Corrected by adding the triplet-singlet hfs mixing contribution, in order to compensate the difference in the definitions of the isotope shift.

[5],  $m/m_h = 1.819\,543\,0761\,(17) \times 10^{-4}$  and  $m/m_\alpha = 1.370\,933\,555\,78\,(55) \times 10^{-4}$ . The first four lines of the tables display the numerical results for the nonrelativistic ( $\sim \alpha^2$ ) recoil corrections given by Eqs. (9), (10), (11), and (12), respectively. The next three lines of the tables contain the results for the relativistic ( $\sim \alpha^4$ ) recoil corrections given by Eqs. (14), (15), and (17)–(20), respectively. The eighth line of the tables contain the QED ( $\sim \alpha^5$ ) recoil corrections given by Eqs. (24)–(26). The line labeled as  $m\alpha^6 m/M$  contains the hydrogenic approximation of the higher-order QED effects as given by Eq. (27). The uncertainty ascribed to this correction represents our estimation of the uncalculated QED effects of order  $\alpha^6$  and higher. Finally, the lines labelled as “Hfsmix” and “NPol” contain the hyperfine mixing correction defined by Eq. (28) and the nuclear polarizability correction given by Eq. (30), respectively.

The uncertainty of the total theoretical values of the isotope shift for the point-like nucleus comes from the uncalculated higher-order QED effects. Note that our estimation of this uncertainty is much larger than the one reported previously in Ref. [1].

The difference of the theoretical point-nucleus values and the experimental isotope shift results should come solely from the finite nuclear size effect. The finite nuclear size correction to the centroid energy can be parameterized as

$$E_{fs} = C R^2, \quad (34)$$

with  $C$  being a coefficient to be calculated numerically. According Eq. (31), the coefficient  $C$  has some dependence on  $R$ , but it is very weak and can be neglected at the level of present interest.

The results of our calculations of the coefficient  $C$  for the  ${}^3\text{He}$ – ${}^4\text{He}$  isotope shift of the  $2^3P$ – $2^3S$  and  $2^1S$ – $2^3S$

TABLE II:  ${}^3\text{He}$ – ${}^4\text{He}$  isotope shift of the  $2^3S - 2^3P$  transition, for the point-like nucleus, in kHz.

$\mu\alpha^2$	12 412 458.1
$\mu\alpha^2 (\mu/M)$	21 243 041.3
$\mu\alpha^2 (\mu/M)^2$	13 874.6
$\mu\alpha^2 (\mu/M)^3$	4.6
$\mu\alpha^4$	17 872.8
$\mu\alpha^4 (\mu/M)$	−20 082.4
$\mu\alpha^4 (\mu/M)^2$	−3.0
$m\alpha^5 (m/M)$	−60.7
$m\alpha^6 (m/M)$	−15.5 (3.9)
Hfsmix	54.6
NPol	−1.1 (1)
Sum	33 667 143.2 (3.9)
Ref. [1] <sup>a</sup>	33 667 146.2 (7)

<sup>a</sup> Corrected by adding the triplet-singlet hfs mixing contribution, in order to compensate the difference in the definitions of the isotope shift.

transition (centroid) energies are

$$C(2^3P - 2^3S) = -1212.2(1) \text{ kHz/fm}^2, \quad (35)$$

$$C(2^1S - 2^3S) = -214.66(2) \text{ kHz/fm}^2. \quad (36)$$

These results can be compared with the previously reported values  $C(2^3P - 2^3S) = -1209.8$  [1] and  $C(2^1S - 2^3S) = -214.40$  [21].

#### IV. NUCLEAR CHARGE RADII DIFFERENCE

We now turn to the determination of the nuclear charge radii difference from the isotope shift. Specifically, by comparing theoretical and experimental values of the centroid energies of different transitions in  ${}^3\text{He}$  and  ${}^4\text{He}$ , we extract the difference of the squares of the nuclear charge radii,

$$\delta R^2 = R^2({}^3\text{He}) - R^2({}^4\text{He}). \quad (37)$$

Using the experimental results for the  $2^1S - 2^3S$  transition energies in  ${}^3\text{He}$  and  ${}^4\text{He}$  from Ref. [2] and taking into account the experimental hyperfine shift of the  $2^3S_1$  state, we obtain  $\delta R^2$  as described in Table III. The results is

$$\delta R^2[\text{Rooij 2011}] = 1.028(11) \text{ fm}^2. \quad (38)$$

This value is somewhat different from the original result of Ref. [2],  $\delta R^2 = 1.019(11) \text{ fm}^2$  because of the updated theoretical prediction for the  $2^1S - 2^3S$  isotope shift (see Table I).

The second experiment on the helium isotope shift suitable for the determination of  $\delta R^2$  is the measurement of the  $2^3P$ – $2^3S$  transition energies in  ${}^3\text{He}$  and  ${}^4\text{He}$  in Refs. [3, 4]. Using these experimental values and the



theory summarized in Table II, we obtain (see Table IV for details)

$$\delta R^2[\text{Cancio 2012}] = 1.074(4) \text{ fm}^2, \quad (39)$$

which deviates from the result (38) by about  $4\sigma$ .

The third experiment that can be used for the determination of  $\delta R^2$  with comparable accuracy is the measurement of the isotope shift difference  $E(^3\text{He}, 2^3P_0^{1/2} - 2^3S_1^{3/2}) - E(^4\text{He}, 2^3P_2 - 2^3S_1)$  performed Ref. [11]. In this experiment, centroid transition energies were not measured, so further theoretical and experimental input is required to extract the charge radii difference  $\delta R^2$ . In order to deduce the experimental value for the isotope shift of the  $2^3P-2^3S$  centroid energy, we subtract from the experimental result of Ref. [11] the experimental hyperfine shift  $\delta E_{\text{hfs}}(2^3S_1^{3/2})$ , theoretical fine shift  $\delta E_{\text{fs}}(2^3P_0)$ , and the theoretical fine and hyperfine shift  $\delta E_{\text{hfs}}(2^3P_0^{1/2})$ . Having obtained the isotope shift of the  $2^3P-2^3S$  centroid energy, we deduce the charge radii difference  $\delta R^2$  with the help of the theory in Table II. The whole determination is summarized in Table V. The result is

$$\delta R^2[\text{Shiner 95}] = 1.066(4) \text{ fm}^2. \quad (40)$$

We observe that the two results from the  $2^3P - 2^3S$  transitions, (39) and (40), are in reasonable (although, marginal) agreement with each other, but deviate significantly from the result deduced from the  $2^1S - 2^3S$  transition (38). The reason of this discrepancy is not known at present.

## V. CONCLUSION

In the present work we have summarized the theory of the isotope shift of the centroid energies of light few-electron atoms. Numerical results are reported for the isotope shift of the  $2^3P-2^3S$  and  $2^1S-2^3S$  transition energies in  $^3\text{He}$  and  $^4\text{He}$ . As compared to the previous evaluations [1, 20], the higher-order recoil  $[\mu\alpha^2(\mu/M)^3]$  and  $\mu\alpha^4(\mu/M)^2$  and the nuclear polarizability corrections were accounted for and the higher-order QED effects  $[m\alpha^6(m/M)]$  were estimated more carefully. By comparing the theoretical predictions with the experimental results for the isotope shift, we have determined the difference of the squares of the nuclear charge radii of  $^3\text{He}$  and  $^4\text{He}$ ,  $\delta R^2$ . The results for  $\delta R^2$  derived from the  $2^3P-2^3S$  and  $2^1S-2^3S$  transitions are shown to disagree with each other by about 4 standard deviations. The reason of this disagreement is presently not known.

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TABLE III: Determination of the charge radii difference  $\delta R^2$  from the measurement by Rooij *et al.* in Ref. [2], in kHz. The remainder  $\delta E$  is proportional to  $\delta R^2$ ,  $\delta E = C \delta R^2$ , with the coefficient  $C$  given by Eq. (35), see text.

$E(^3\text{He}, 2^1S^{F=1/2} - 2^3S^{F=3/2}) - E(^4\text{He}, 2^1S - 2^3S)$	$-5\,787\,719.2(2.4)$	Exp. [2]
$\delta E_{\text{hfs}}(2^3S^{3/2})$	$-2\,246\,567.059(5)$	Exp. [22, 23]
$-\delta E_{\text{iso}}(2^1S - 2^3S)$ (point nucleus)	$8\,034\,065.66(69)$	Theory, Table I
$\delta E$	$-220.6(2.4)$	

TABLE IV: Determination of the charge radii difference  $\delta R^2$  from the measurements by Cancio Pastor *et al.* in Refs. [3, 4], in kHz. The remainder  $\delta E$  is proportional to  $\delta R^2$ ,  $\delta E = C \delta R^2$ , with the coefficient  $C$  given by Eq. (36), see text.

$E(^3\text{He}, 2^3P - 2S)$ (centroid)	$276\,702\,827\,204.8(2.4)$	Exp. [3]
$-E(^4\text{He}, 2^3P - 2S)$ (centroid)	$-276\,736\,495\,649.5(2.1)$	Exp. [4, 24] <sup>a</sup>
$-\delta E_{\text{iso}}(2^3P - 2^3S)$ (point nucleus)	$33\,667\,143.2(3.9)$	Theory, Table II
$\delta E$	$-1\,301.5(5.0)$	

<sup>a</sup> obtained by combining the  $2^3S_1 - 2^3P_{0,1}$  transition energies from Ref. [4] and the  $2^3P_0 - 2^3P_2$  energy from Ref. [24].

TABLE V: Determination of the charge radii difference  $\delta R^2$  from the measurement by Shiner *et al.* in [11], in kHz. The remainder  $\delta E$  is proportional to  $\delta R^2$ ,  $\delta E = C \delta R^2$ , with the coefficient  $C$  given by Eq. (36), see text.

$E(^3\text{He}, 2^3P_0^{1/2} - 2^3S_1^{3/2}) - E(^4\text{He}, 2^3P_2 - 2^3S_1)$	$810\,599.0(3.0)$	Exp. [11]
$\delta E_{\text{hfs}}(2^3S_1^{3/2})$	$-2\,246\,567.059(5)$	Exp. [22, 23]
$\delta E_{\text{fs}}(2^3P_2)$	$-4\,309\,074.2(1.7)$	Theory [25]
$-\delta E_{\text{fs,hfs}}(2^3P_0^{1/2})$	$-27\,923\,393.7(1.7)$	Theory [26]
$-\delta E_{\text{iso}}(2^3P - 2^3S)$ (point nucleus)	$33\,667\,143.2(3.9)$	Theory, Table II
$\delta E$	$-1\,292.8(5.2)$	